



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:56 PM UTC

PDB ID : 3NAW / pdb_00003naw
Title : Crystal structure of E. coli O157:H7 effector protein NleL
Authors : Lin, D.Y.; Chen, J.
Deposited on : 2010-06-02
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

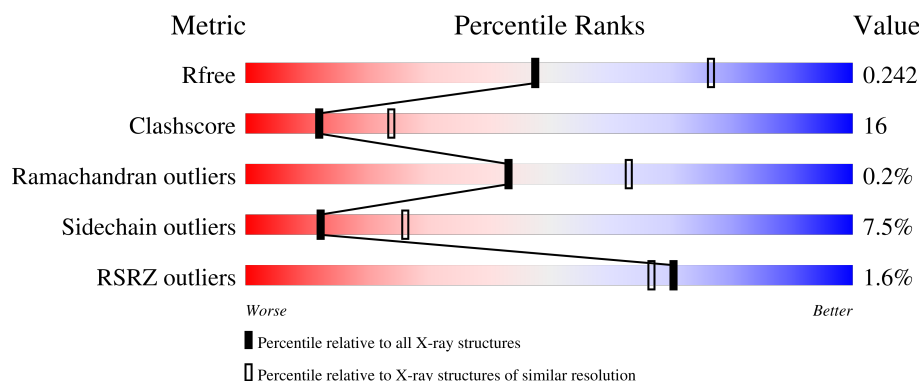
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	613	% 71% 24% ..
1	B	613	2% 67% 28% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10041 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called secreted effector protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4820	3055	780	948	37			
1	B	610	Total	C	N	O	S	2	0	0
			4820	3058	781	944	37			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



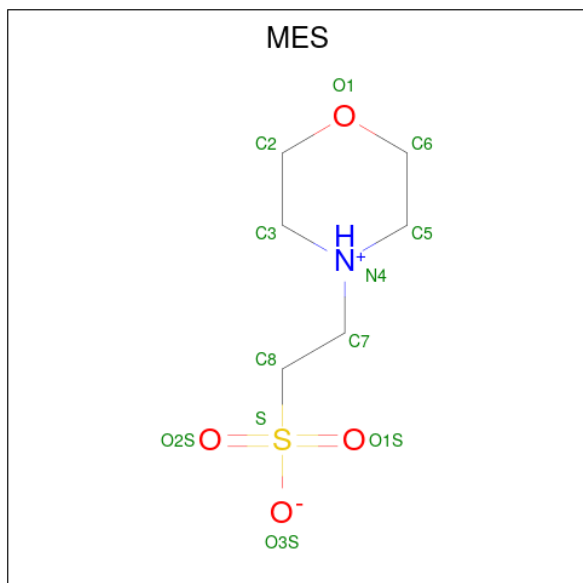
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

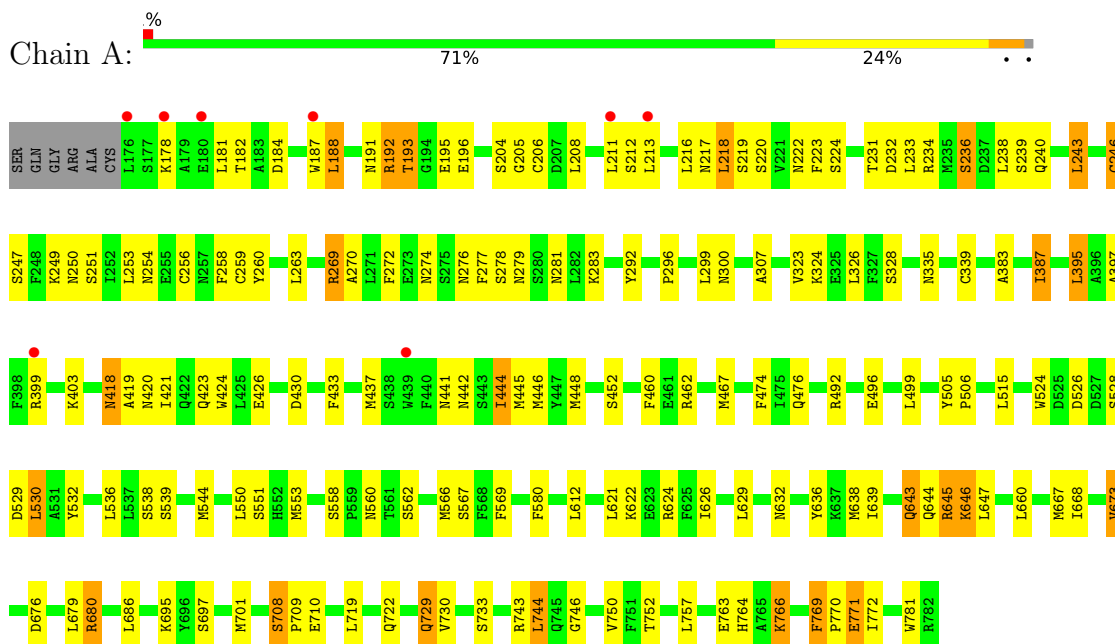
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	B	122	Total	O	0	0
			122	122		

3 Residue-property plots

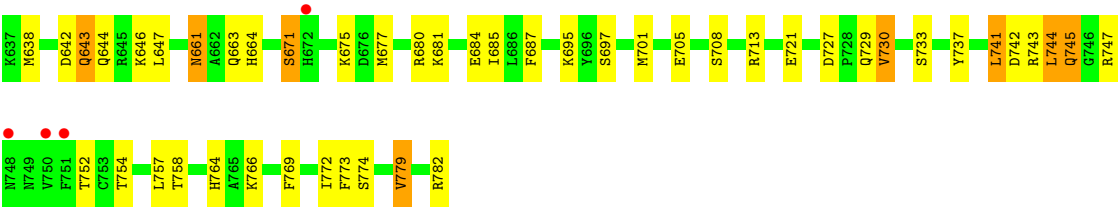
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: secreted effector protein



• Molecule 1: secreted effector protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	313.67Å 77.31Å 61.51Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	47.05 – 2.50 47.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.05-2.50) 98.2 (47.05-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.184 , 0.246 0.181 , 0.242	Depositor DCC
R_{free} test set	3007 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10041	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/4925	0.86	7/6666 (0.1%)
1	B	0.52	0/4925	0.84	3/6667 (0.0%)
All	All	0.54	0/9850	0.85	10/13333 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	769	PHE	CA-C-N	7.88	127.94	119.28
1	A	769	PHE	C-N-CA	7.88	127.94	119.28
1	A	558	SER	CA-C-N	7.56	127.49	119.85
1	A	558	SER	C-N-CA	7.56	127.49	119.85
1	B	194	GLY	N-CA-C	-7.25	104.44	114.67
1	A	708	SER	CA-C-N	6.10	127.46	119.84
1	A	708	SER	C-N-CA	6.10	127.46	119.84
1	B	592	PHE	CA-C-N	5.83	125.50	119.56
1	B	592	PHE	C-N-CA	5.83	125.50	119.56
1	A	668	ILE	CB-CA-C	-5.36	105.03	112.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4820	0	4619	138	0
1	B	4820	0	4609	167	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
3	A	24	0	32	0	0
3	B	30	0	40	4	0
4	B	12	0	12	3	0
5	A	173	0	0	5	0
5	B	122	0	0	4	0
All	All	10041	0	9312	298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:LEU:HG	1:B:458:MET:HE2	1.33	1.10
1:A:643:GLN:HA	1:A:643:GLN:HE21	1.04	1.10
1:A:636:TYR:HE2	1:A:638:MET:HE2	1.18	1.08
1:B:398:PHE:CD1	1:B:400:PRO:HG3	1.92	1.02
1:A:274:ASN:HD21	1:B:316:SER:HB3	1.34	0.92
1:B:708:SER:OG	1:B:713:ARG:HD3	1.71	0.89
1:A:636:TYR:CE2	1:A:638:MET:HE2	2.07	0.88
1:B:680:ARG:HE	1:B:729:GLN:HE21	1.21	0.86
1:B:680:ARG:O	1:B:684:GLU:HG3	1.75	0.85
1:B:695:LYS:HD3	1:B:758:THR:HG21	1.56	0.84
1:B:741:LEU:O	1:B:745:GLN:HG3	1.78	0.84
1:A:643:GLN:HA	1:A:643:GLN:NE2	1.85	0.81
1:B:197:SER:HB2	1:B:200:GLU:HB2	1.63	0.81
1:B:263:LEU:O	1:B:266:CYS:HB2	1.81	0.81
1:A:448:MET:CE	1:A:452:SER:HB3	2.11	0.81
1:A:448:MET:HE2	1:A:452:SER:HB3	1.63	0.81
1:A:213:LEU:HB3	1:A:216:LEU:HD12	1.65	0.78
1:A:188:LEU:HD22	1:A:192:ARG:HD3	1.66	0.78
1:B:328:SER:HB2	1:B:335:ASN:OD1	1.85	0.77
1:A:233:LEU:O	1:A:236:SER:HB2	1.85	0.76
1:A:433:PHE:CE1	1:A:448:MET:HE1	2.20	0.76
1:A:281:ASN:HD21	1:A:283:LYS:HD3	1.50	0.76
1:A:560:ASN:HB3	1:A:562:SER:H	1.52	0.75
1:B:211:LEU:HD13	1:B:213:LEU:HG	1.67	0.74
1:A:643:GLN:HE21	1:A:643:GLN:CA	1.93	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:GLN:HE21	1:B:643:GLN:N	1.85	0.74
1:A:418:ASN:ND2	1:A:421:ILE:H	1.86	0.72
1:B:325:GLU:HB3	5:B:811:HOH:O	1.89	0.72
1:B:208:LEU:HD12	1:B:211:LEU:HD21	1.70	0.72
1:B:680:ARG:NE	1:B:729:GLN:HE21	1.87	0.72
1:A:433:PHE:HE1	1:A:448:MET:HE1	1.53	0.71
1:A:279:ASN:HD21	1:B:257:ASN:HD21	1.38	0.71
1:B:178:LYS:NZ	1:B:209:SER:HB3	2.06	0.70
1:A:243:LEU:O	1:A:246:CYS:HB2	1.92	0.70
1:B:398:PHE:CE1	1:B:400:PRO:HG3	2.26	0.70
1:B:455:GLN:HA	1:B:458:MET:HE3	1.74	0.69
1:B:680:ARG:HE	1:B:729:GLN:NE2	1.90	0.68
1:B:680:ARG:NH2	1:B:729:GLN:HG3	2.08	0.68
1:B:697:SER:O	1:B:708:SER:HB2	1.93	0.68
1:B:299:LEU:HD13	1:B:304:LEU:HD11	1.74	0.68
1:B:264:SER:HB3	1:B:281:ASN:OD1	1.93	0.68
1:B:281:ASN:HD21	1:B:283:LYS:HD3	1.59	0.66
1:A:418:ASN:HD22	1:A:421:ILE:H	1.42	0.66
1:B:213:LEU:HB2	1:B:233:LEU:HD23	1.77	0.66
1:B:176:LEU:HD23	1:B:177:SER:H	1.62	0.65
1:A:638:MET:HA	1:A:643:GLN:HG2	1.77	0.65
1:A:274:ASN:ND2	1:B:316:SER:HB3	2.10	0.65
1:B:445:MET:H	1:B:476:GLN:NE2	1.94	0.65
1:A:771:GLU:H	1:A:771:GLU:CD	2.05	0.65
1:A:638:MET:HA	1:A:643:GLN:CG	2.26	0.64
1:A:448:MET:HE2	1:A:452:SER:C	2.23	0.64
1:B:661:ASN:ND2	1:B:664:HIS:H	1.96	0.63
1:A:528:SER:OG	1:A:530:LEU:HD22	1.98	0.62
1:A:492:ARG:O	1:A:496:GLU:HG3	1.99	0.62
1:B:766:LYS:HE2	1:B:773:PHE:CE2	2.34	0.62
1:A:253:LEU:HD22	1:A:258:PHE:HZ	1.65	0.62
1:A:292:TYR:CZ	1:A:296:PRO:HB3	2.35	0.61
1:A:251:SER:O	1:A:270:ALA:HB1	1.99	0.61
1:A:184:ASP:O	1:A:188:LEU:HB2	2.00	0.61
1:A:279:ASN:HD21	1:B:257:ASN:ND2	1.97	0.61
1:B:234:ARG:HD3	4:B:1:MES:H21	1.82	0.61
1:A:383:ALA:O	1:A:387:ILE:HG23	2.01	0.61
1:B:231:THR:HG22	1:B:233:LEU:HG	1.83	0.60
1:A:204:SER:C	1:A:206:CYS:H	2.08	0.60
1:A:730:VAL:O	1:A:764:HIS:HE1	1.84	0.60
1:A:744:LEU:HD13	1:A:757:LEU:CD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:HD21	1:A:420:ASN:HB3	1.67	0.59
1:A:178:LYS:HG2	5:A:803:HOH:O	2.02	0.59
1:A:529:ASP:HA	5:A:864:HOH:O	2.01	0.59
1:A:526:ASP:OD1	1:A:528:SER:HB3	2.03	0.59
1:B:528:SER:HB2	1:B:530:LEU:HD23	1.84	0.59
1:A:192:ARG:HD2	1:A:196:GLU:OE1	2.02	0.59
1:B:467:MET:HE3	1:B:494:LEU:HD11	1.85	0.58
1:A:239:SER:O	1:A:240:GLN:HB2	2.03	0.58
1:A:277:PHE:HB2	1:A:299:LEU:HD23	1.85	0.58
1:A:566:MET:HE3	1:A:580:PHE:CZ	2.38	0.58
1:B:536:LEU:HD11	1:B:553:MET:HE1	1.86	0.58
1:A:433:PHE:HE1	1:A:448:MET:CE	2.16	0.58
1:B:178:LYS:HZ1	1:B:209:SER:HB3	1.66	0.58
1:B:221:VAL:HG11	1:B:223:PHE:CZ	2.39	0.58
1:B:208:LEU:HB3	1:B:211:LEU:HD21	1.86	0.58
1:A:208:LEU:O	1:A:211:LEU:HG	2.04	0.57
1:A:528:SER:OG	1:A:530:LEU:HB2	2.04	0.57
1:A:419:ALA:O	1:A:423:GLN:HG3	2.04	0.57
1:B:350:ILE:O	1:B:353:VAL:HG22	2.04	0.57
1:B:237:ASP:OD1	1:B:237:ASP:C	2.47	0.56
1:B:628:ALA:HB1	1:B:701:MET:CE	2.35	0.56
1:B:595:PHE:O	1:B:598:PRO:HD2	2.05	0.56
1:B:479:MET:HE1	1:B:553:MET:SD	2.45	0.56
1:A:232:ASP:OD1	1:A:234:ARG:HG3	2.05	0.56
1:A:766:LYS:O	1:A:770:PRO:HG3	2.05	0.56
1:B:185:LEU:HD13	1:B:186:ILE:N	2.21	0.56
1:A:744:LEU:HD13	1:A:757:LEU:HD21	1.88	0.56
1:B:779:VAL:O	1:B:782:ARG:HG2	2.06	0.56
1:B:528:SER:O	1:B:529:ASP:HB2	2.06	0.56
1:B:186:ILE:HD13	1:B:186:ILE:O	2.06	0.55
1:A:467:MET:HG2	1:A:474:PHE:CE1	2.42	0.55
1:B:307:ALA:O	1:B:339:CYS:HB2	2.07	0.55
1:B:727:ASP:OD1	1:B:729:GLN:HG2	2.06	0.55
1:B:742:ASP:HA	1:B:747:ARG:HG3	1.89	0.55
1:B:730:VAL:O	1:B:764:HIS:HE1	1.89	0.55
1:B:305:THR:HG23	1:B:321:GLY:HA3	1.89	0.54
1:A:645:ARG:HH11	1:A:645:ARG:HB2	1.72	0.54
1:B:211:LEU:CD1	1:B:231:THR:HG23	2.37	0.54
1:B:300:ASN:H	1:B:300:ASN:HD22	1.55	0.54
1:A:567:SER:HB3	5:A:817:HOH:O	2.07	0.54
1:B:445:MET:H	1:B:476:GLN:HE22	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:ARG:O	1:B:752:THR:HG23	2.08	0.54
1:A:217:ASN:C	1:A:218:LEU:HD23	2.33	0.54
1:B:323:VAL:HG21	1:B:326:LEU:HD23	1.90	0.54
1:B:721:GLU:HG3	1:B:737:TYR:OH	2.08	0.54
1:A:259:CYS:O	1:A:260:TYR:HB2	2.07	0.53
1:B:255:GLU:OE1	4:B:1:MES:H82	2.08	0.53
1:B:181:LEU:HD22	1:B:206:CYS:SG	2.49	0.53
1:B:661:ASN:HD21	1:B:663:GLN:HB3	1.75	0.53
1:B:204:SER:HB3	1:B:222:ASN:HD21	1.74	0.52
1:A:278:SER:O	1:A:279:ASN:HB2	2.09	0.52
1:A:397:ALA:HB3	1:A:399:ARG:CG	2.39	0.52
1:B:628:ALA:HB1	1:B:701:MET:HE1	1.90	0.52
1:A:445:MET:H	1:A:476:GLN:NE2	2.07	0.52
1:A:243:LEU:HD12	1:A:263:LEU:HD21	1.91	0.52
1:A:448:MET:HE3	1:A:452:SER:HB3	1.90	0.52
1:A:673:VAL:HG13	5:A:84:HOH:O	2.09	0.52
1:A:746:GLY:HA2	1:A:750:VAL:O	2.09	0.52
1:B:325:GLU:OE2	1:B:328:SER:HA	2.09	0.52
1:B:357:TYR:CE1	3:B:783:GOL:H32	2.44	0.51
1:B:219:SER:O	1:B:220:SER:HB2	2.09	0.51
1:A:258:PHE:HB2	1:A:276:ASN:O	2.11	0.51
1:B:744:LEU:HD13	1:B:757:LEU:CD2	2.40	0.51
1:B:528:SER:HB2	1:B:530:LEU:CD2	2.39	0.51
1:B:233:LEU:O	1:B:236:SER:HB2	2.10	0.51
1:B:253:LEU:O	1:B:256:CYS:HB2	2.11	0.50
1:B:437:MET:CE	1:B:456:ALA:HB1	2.41	0.50
1:A:399:ARG:O	1:A:403:LYS:HD3	2.12	0.50
1:B:211:LEU:HD12	1:B:231:THR:HG23	1.93	0.50
1:A:323:VAL:HG11	1:A:326:LEU:HD23	1.93	0.50
1:A:445:MET:H	1:A:476:GLN:HE22	1.60	0.50
1:A:566:MET:CE	1:A:580:PHE:CE1	2.94	0.50
1:B:743:ARG:HD2	1:B:757:LEU:HD13	1.92	0.50
1:B:208:LEU:HD12	1:B:211:LEU:CD2	2.41	0.49
1:B:217:ASN:N	1:B:217:ASN:OD1	2.45	0.49
1:B:530:LEU:N	1:B:530:LEU:HD22	2.27	0.49
1:A:528:SER:O	1:A:530:LEU:HD13	2.12	0.49
1:A:660:LEU:HD11	1:A:719:LEU:HD23	1.93	0.49
1:B:208:LEU:O	1:B:211:LEU:HG	2.12	0.49
1:B:221:VAL:CG1	1:B:223:PHE:CZ	2.95	0.49
1:B:528:SER:CB	1:B:530:LEU:HD23	2.42	0.49
1:A:307:ALA:O	1:A:339:CYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:SER:O	1:A:708:SER:HB2	2.12	0.49
1:A:253:LEU:HD22	1:A:258:PHE:CZ	2.45	0.49
1:B:644:GLN:NE2	5:B:844:HOH:O	2.46	0.48
1:A:328:SER:HB2	1:A:335:ASN:OD1	2.12	0.48
1:B:376:ASN:CG	1:B:414:PRO:HG3	2.39	0.48
1:B:684:GLU:HG2	1:B:730:VAL:HG22	1.94	0.48
1:A:274:ASN:HD21	1:B:316:SER:CB	2.18	0.48
1:B:208:LEU:HB2	1:B:227:VAL:O	2.13	0.48
1:B:499:LEU:HD21	1:B:522:PRO:HG3	1.95	0.48
1:A:638:MET:HA	1:A:643:GLN:HG3	1.94	0.48
1:B:430:ASP:O	1:B:434:ASP:HB2	2.14	0.48
1:A:213:LEU:CB	1:A:216:LEU:HD12	2.40	0.48
1:B:197:SER:O	1:B:198:ALA:C	2.56	0.48
1:B:343:LEU:HD21	1:B:364:ILE:HD12	1.96	0.48
1:A:643:GLN:NE2	1:A:646:LYS:HE3	2.29	0.48
1:A:233:LEU:O	1:A:256:CYS:SG	2.72	0.47
1:A:426:GLU:O	1:A:430:ASP:HB2	2.14	0.47
1:A:680:ARG:HD3	1:A:729:GLN:OE1	2.14	0.47
1:B:246:CYS:HB2	1:B:266:CYS:SG	2.54	0.47
1:B:217:ASN:C	1:B:219:SER:H	2.22	0.47
1:B:444:ILE:HA	1:B:476:GLN:HE22	1.78	0.47
1:A:233:LEU:O	1:A:234:ARG:C	2.58	0.47
1:B:521:LYS:HA	1:B:521:LYS:HD3	1.60	0.47
1:B:178:LYS:HZ3	1:B:209:SER:HB3	1.76	0.47
1:B:680:ARG:HH21	1:B:729:GLN:HG3	1.80	0.47
1:A:187:TRP:NE1	1:A:191:ASN:ND2	2.63	0.47
1:A:213:LEU:HB2	1:A:233:LEU:HD22	1.97	0.47
1:A:418:ASN:HD22	1:A:418:ASN:C	2.22	0.47
1:A:188:LEU:O	1:A:192:ARG:HG2	2.15	0.47
1:A:448:MET:HE2	1:A:452:SER:CB	2.40	0.47
1:B:221:VAL:HB	1:B:223:PHE:CE2	2.50	0.47
1:B:238:LEU:O	1:B:241:ALA:HB3	2.15	0.46
1:A:243:LEU:HD23	1:A:243:LEU:N	2.30	0.46
1:A:204:SER:C	1:A:206:CYS:N	2.73	0.46
1:B:213:LEU:HB2	1:B:233:LEU:CD2	2.43	0.46
1:A:204:SER:O	1:A:206:CYS:N	2.48	0.46
1:B:203:TYR:O	1:B:206:CYS:HB2	2.16	0.46
1:B:766:LYS:HE3	1:B:766:LYS:HB2	1.60	0.46
1:B:197:SER:HB2	1:B:200:GLU:CB	2.41	0.46
1:A:686:LEU:HD13	1:A:722:GLN:HG3	1.97	0.46
1:B:204:SER:HB3	1:B:222:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:PHE:C	1:B:513:PHE:CD2	2.94	0.45
1:B:608:VAL:HG12	1:B:612:LEU:HD22	1.98	0.45
1:A:418:ASN:ND2	1:A:418:ASN:C	2.74	0.45
1:B:178:LYS:HA	1:B:181:LEU:HD21	1.97	0.45
1:A:247:SER:OG	1:A:249:LYS:HE3	2.16	0.45
1:A:444:ILE:HA	1:A:476:GLN:HE22	1.81	0.45
1:B:730:VAL:O	1:B:764:HIS:CE1	2.70	0.45
1:B:228:LEU:HD13	1:B:248:PHE:CZ	2.52	0.45
1:B:231:THR:CG2	1:B:233:LEU:HG	2.46	0.45
1:B:413:HIS:HD2	5:B:55:HOH:O	2.00	0.45
1:B:269:ARG:O	1:B:269:ARG:HG2	2.16	0.45
1:B:404:MET:SD	1:B:446:MET:HE1	2.56	0.45
1:B:467:MET:HE3	1:B:494:LEU:CD1	2.47	0.45
1:A:538:SER:HB2	1:A:544:MET:HB2	1.99	0.45
1:A:566:MET:HE3	1:A:580:PHE:CE1	2.52	0.45
1:A:769:PHE:N	1:A:770:PRO:HD3	2.31	0.45
1:B:182:THR:HA	1:B:185:LEU:HD12	1.99	0.45
1:B:282:LEU:HB2	1:B:303:ASP:O	2.17	0.45
1:B:233:LEU:O	1:B:234:ARG:C	2.59	0.45
1:B:399:ARG:N	1:B:400:PRO:HD3	2.32	0.45
1:A:218:LEU:HD23	1:A:218:LEU:N	2.32	0.44
1:B:467:MET:CE	1:B:494:LEU:CD1	2.95	0.44
1:A:192:ARG:NH2	1:A:219:SER:O	2.51	0.44
1:A:744:LEU:HD13	1:A:757:LEU:HD23	1.99	0.44
1:A:445:MET:HG3	1:A:446:MET:O	2.18	0.44
1:A:279:ASN:ND2	1:B:257:ASN:HD21	2.09	0.44
1:B:586:ASN:HB3	1:B:590:GLU:OE1	2.18	0.44
1:B:744:LEU:HD13	1:B:757:LEU:HD23	1.98	0.44
1:B:185:LEU:HD11	1:B:213:LEU:HD22	1.99	0.44
1:B:631:SER:C	1:B:633:LYS:H	2.25	0.44
1:A:219:SER:O	1:A:220:SER:HB2	2.17	0.43
1:B:595:PHE:C	1:B:598:PRO:HD2	2.42	0.43
1:B:177:SER:HB3	1:B:180:GLU:CB	2.47	0.43
1:B:418:ASN:HD22	1:B:421:ILE:H	1.65	0.43
1:B:599:TYR:OH	3:B:9:GOL:H11	2.18	0.43
1:A:233:LEU:HD13	1:A:238:LEU:HD11	1.99	0.43
1:A:532:TYR:CZ	1:A:569:PHE:HE2	2.36	0.43
1:B:254:ASN:HD22	4:B:1:MES:C6	2.31	0.43
1:A:772:ILE:HD13	1:A:772:ILE:HA	1.80	0.43
1:A:397:ALA:HB3	1:A:399:ARG:HG2	1.99	0.43
1:A:701:MET:HE3	1:A:701:MET:HB3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:MET:HA	1:B:571:TYR:O	2.18	0.43
1:B:752:THR:HG22	1:B:754:THR:HG23	2.01	0.43
1:A:222:ASN:OD1	1:A:222:ASN:C	2.61	0.43
1:A:695:LYS:HG2	1:A:781:TRP:CE3	2.54	0.43
1:B:687:PHE:C	1:B:687:PHE:CD2	2.97	0.43
1:A:178:LYS:HD3	1:A:181:LEU:HD21	1.99	0.43
1:A:492:ARG:HG2	1:A:524:TRP:CE2	2.53	0.43
1:B:552:HIS:CE1	1:B:556:MET:SD	3.11	0.43
1:A:231:THR:H	1:A:251:SER:HB3	1.82	0.43
1:B:221:VAL:CG1	1:B:223:PHE:CE2	3.01	0.43
1:B:325:GLU:O	1:B:325:GLU:HG3	2.18	0.43
1:B:300:ASN:HD22	1:B:300:ASN:N	2.16	0.42
1:A:278:SER:CB	1:B:276:ASN:HD21	2.32	0.42
1:B:632:ASN:C	1:B:633:LYS:HG2	2.43	0.42
1:B:677:MET:SD	1:B:685:ILE:CD1	3.07	0.42
1:A:223:PHE:O	1:A:224:SER:C	2.62	0.42
1:A:250:ASN:OD1	1:A:269:ARG:HD2	2.20	0.42
1:A:679:LEU:O	1:A:680:ARG:C	2.62	0.42
1:B:299:LEU:HD12	1:B:315:LEU:HD23	2.01	0.42
1:B:437:MET:HE1	1:B:477:ILE:HG13	2.01	0.42
1:B:192:ARG:HD2	1:B:192:ARG:HA	1.88	0.42
1:B:553:MET:HE3	1:B:553:MET:HB2	1.63	0.42
1:A:639:ILE:O	1:A:644:GLN:NE2	2.51	0.42
1:A:667:MET:HE2	1:A:667:MET:HA	2.00	0.42
1:B:185:LEU:C	1:B:185:LEU:HD22	2.45	0.42
1:B:235:MET:HE3	1:B:235:MET:HB2	1.95	0.42
1:B:244:GLU:HB2	1:B:262:ASN:ND2	2.34	0.42
1:B:350:ILE:HD12	1:B:350:ILE:HA	1.89	0.42
1:A:324:LYS:HG2	5:A:823:HOH:O	2.20	0.42
1:B:192:ARG:HH21	1:B:194:GLY:H	1.66	0.42
1:A:387:ILE:HD12	1:A:424:TRP:CD1	2.54	0.42
1:B:482:SER:O	1:B:488:GLN:HG2	2.20	0.42
1:A:395:LEU:HD12	1:A:395:LEU:HA	1.78	0.41
1:B:223:PHE:O	1:B:224:SER:C	2.63	0.41
1:B:357:TYR:CD1	3:B:783:GOL:H32	2.55	0.41
1:B:626:ILE:O	1:B:629:LEU:HB2	2.20	0.41
1:A:260:TYR:CZ	1:A:279:ASN:ND2	2.88	0.41
1:A:730:VAL:HG13	1:A:769:PHE:CE2	2.55	0.41
1:B:199:GLU:HB3	1:B:202:ASN:ND2	2.35	0.41
1:B:499:LEU:HD12	1:B:499:LEU:HA	1.77	0.41
1:A:445:MET:HB2	1:A:445:MET:HE2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:LEU:O	1:A:624:ARG:HB2	2.20	0.41
1:B:492:ARG:HG2	1:B:524:TRP:CE2	2.55	0.41
1:B:631:SER:C	1:B:633:LYS:N	2.77	0.41
1:B:671:SER:O	1:B:675:LYS:HB3	2.21	0.41
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.93	0.41
1:B:772:ILE:HD13	1:B:772:ILE:HA	1.93	0.41
1:A:430:ASP:OD1	1:A:462:ARG:NH2	2.29	0.41
1:B:638:MET:SD	1:B:647:LEU:HD11	2.60	0.41
1:B:201:LEU:HA	1:B:203:TYR:CE2	2.56	0.41
1:B:478:VAL:HG11	1:B:495:TYR:HB2	2.03	0.41
1:B:684:GLU:HB3	1:B:769:PHE:CD1	2.56	0.41
1:B:204:SER:C	1:B:206:CYS:H	2.28	0.41
1:A:300:ASN:HD22	1:A:300:ASN:H	1.69	0.41
1:A:441:ASN:O	1:A:442:ASN:HB2	2.21	0.41
1:A:505:TYR:N	1:A:506:PRO:CD	2.84	0.41
1:A:181:LEU:HD12	1:A:182:THR:N	2.36	0.41
1:A:212:SER:HB2	1:A:232:ASP:HB3	2.03	0.41
1:A:708:SER:HA	1:A:709:PRO:HD3	1.85	0.40
1:A:743:ARG:HH11	1:A:752:THR:HG21	1.86	0.40
1:A:253:LEU:O	1:A:254:ASN:C	2.64	0.40
1:A:437:MET:HG2	1:A:460:PHE:CZ	2.55	0.40
1:A:530:LEU:HD12	1:A:551:SER:HB3	2.02	0.40
1:A:193:THR:HG23	1:A:196:GLU:CD	2.47	0.40
1:B:248:PHE:HB2	1:B:268:ILE:HA	2.03	0.40
1:B:610:GLY:HA3	5:B:819:HOH:O	2.21	0.40
1:B:193:THR:C	1:B:195:GLU:H	2.29	0.40
1:B:439:TRP:CH2	3:B:5:GOL:H31	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	605/613 (99%)	574 (95%)	30 (5%)	1 (0%)	43 63
1	B	608/613 (99%)	550 (90%)	56 (9%)	2 (0%)	36 55
All	All	1213/1226 (99%)	1124 (93%)	86 (7%)	3 (0%)	43 63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	210	GLY
1	B	671	SER
1	A	205	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	540/546 (99%)	500 (93%)	40 (7%)	13 27
1	B	535/546 (98%)	494 (92%)	41 (8%)	12 25
All	All	1075/1092 (98%)	994 (92%)	81 (8%)	12 26

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LEU
1	A	192	ARG
1	A	193	THR
1	A	195	GLU
1	A	218	LEU
1	A	236	SER
1	A	243	LEU
1	A	246	CYS
1	A	269	ARG
1	A	272	PHE
1	A	387	ILE
1	A	395	LEU
1	A	418	ASN

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Mol	Chain	Res	Type
1	A	444	ILE
1	A	499	LEU
1	A	515	LEU
1	A	530	LEU
1	A	536	LEU
1	A	539	SER
1	A	550	LEU
1	A	553	MET
1	A	612	LEU
1	A	622	LYS
1	A	626	ILE
1	A	629	LEU
1	A	632	ASN
1	A	643	GLN
1	A	645	ARG
1	A	646	LYS
1	A	647	LEU
1	A	673	VAL
1	A	676	ASP
1	A	680	ARG
1	A	710	GLU
1	A	729	GLN
1	A	733	SER
1	A	744	LEU
1	A	763	GLU
1	A	766	LYS
1	A	771	GLU
1	B	176	LEU
1	B	185	LEU
1	B	186	ILE
1	B	192	ARG
1	B	199	GLU
1	B	201	LEU
1	B	217	ASN
1	B	227	VAL
1	B	236	SER
1	B	265	ASN
1	B	266	CYS
1	B	267	ILE
1	B	272	PHE
1	B	305	THR
1	B	323	VAL

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Mol	Chain	Res	Type
1	B	345	ASP
1	B	395	LEU
1	B	411	SER
1	B	430	ASP
1	B	472	SER
1	B	499	LEU
1	B	527	ASP
1	B	553	MET
1	B	584	LEU
1	B	594	ILE
1	B	612	LEU
1	B	627	GLU
1	B	629	LEU
1	B	642	ASP
1	B	643	GLN
1	B	646	LYS
1	B	661	ASN
1	B	681	LYS
1	B	705	GLU
1	B	730	VAL
1	B	733	SER
1	B	741	LEU
1	B	744	LEU
1	B	745	GLN
1	B	774	SER
1	B	779	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	245	ASN
1	A	274	ASN
1	A	279	ASN
1	A	281	ASN
1	A	294	GLN
1	A	300	ASN
1	A	418	ASN
1	A	476	GLN
1	A	480	ASN
1	A	509	GLN
1	A	552	HIS

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Mol	Chain	Res	Type
1	A	577	GLN
1	A	606	ASN
1	A	632	ASN
1	A	643	GLN
1	A	682	GLN
1	A	722	GLN
1	A	729	GLN
1	A	749	ASN
1	A	764	HIS
1	B	240	GLN
1	B	245	ASN
1	B	254	ASN
1	B	281	ASN
1	B	284	ASN
1	B	347	GLN
1	B	420	ASN
1	B	442	ASN
1	B	476	GLN
1	B	509	GLN
1	B	540	GLN
1	B	577	GLN
1	B	600	HIS
1	B	606	ASN
1	B	619	ASN
1	B	643	GLN
1	B	661	ASN
1	B	717	ASN
1	B	729	GLN
1	B	745	GLN
1	B	764	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	5	-	4,4,4	0.23	0	6,6,6	0.10	0
3	GOL	A	784	-	5,5,5	0.45	0	5,5,5	0.33	0
2	SO4	A	1	-	4,4,4	0.17	0	6,6,6	0.24	0
3	GOL	A	8	-	5,5,5	0.34	0	5,5,5	0.32	0
2	SO4	B	7	-	4,4,4	0.18	0	6,6,6	0.20	0
3	GOL	B	783	-	5,5,5	0.41	0	5,5,5	0.49	0
3	GOL	B	9	-	5,5,5	0.37	0	5,5,5	0.73	0
4	MES	B	1	-	12,12,12	2.30	1 (8%)	15,16,16	2.56	7 (46%)
2	SO4	A	3	-	4,4,4	0.24	0	6,6,6	0.15	0
3	GOL	B	3	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	A	783	-	5,5,5	0.35	0	5,5,5	0.22	0
2	SO4	B	8	-	4,4,4	0.25	0	6,6,6	0.11	0
3	GOL	B	5	-	5,5,5	0.35	0	5,5,5	0.30	0
3	GOL	B	6	-	5,5,5	0.36	0	5,5,5	0.44	0
2	SO4	B	10	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	A	4	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.15	0
3	GOL	A	7	-	5,5,5	0.38	0	5,5,5	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	784	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	783	-	-	2/4/4/4	-
3	GOL	A	8	-	-	2/4/4/4	-
3	GOL	B	9	-	-	2/4/4/4	-
4	MES	B	1	-	-	1/6/14/14	0/1/1/1
3	GOL	B	3	-	-	2/4/4/4	-
3	GOL	A	783	-	-	1/4/4/4	-
3	GOL	B	5	-	-	3/4/4/4	-
3	GOL	B	6	-	-	4/4/4/4	-
3	GOL	A	7	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	MES	C8-S	-7.70	1.66	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	MES	C5-N4-C3	4.79	119.16	108.84
4	B	1	MES	C2-C3-N4	-4.05	103.96	110.12
4	B	1	MES	C7-N4-C3	3.78	121.30	111.24
4	B	1	MES	C6-C5-N4	-3.72	104.47	110.12
4	B	1	MES	C7-N4-C5	3.11	119.53	111.24
4	B	1	MES	O1S-S-C8	2.12	109.93	106.73
4	B	1	MES	O3S-S-C8	2.01	109.93	106.00

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	784	GOL	O1-C1-C2-C3
3	A	8	GOL	O1-C1-C2-C3
3	B	783	GOL	O1-C1-C2-C3
3	B	6	GOL	C1-C2-C3-O3
3	B	9	GOL	O1-C1-C2-C3
3	A	784	GOL	O1-C1-C2-O2
3	B	6	GOL	O1-C1-C2-O2
3	A	784	GOL	C1-C2-C3-O3
3	B	3	GOL	C1-C2-C3-O3
3	B	5	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	6	GOL	O1-C1-C2-C3
3	A	8	GOL	O1-C1-C2-O2
3	B	6	GOL	O2-C2-C3-O3
3	B	9	GOL	O1-C1-C2-O2
3	B	783	GOL	O1-C1-C2-O2
3	A	784	GOL	O2-C2-C3-O3
3	B	3	GOL	O2-C2-C3-O3
3	A	783	GOL	O1-C1-C2-O2
3	B	5	GOL	O2-C2-C3-O3
4	B	1	MES	C8-C7-N4-C3
3	B	5	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	783	GOL	2	0
3	B	9	GOL	1	0
4	B	1	MES	3	0
3	B	5	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	607/613 (99%)	-0.16	8 (1%) 75 71	26, 52, 112, 177	2 (0%)
1	B	610/613 (99%)	-0.01	12 (1%) 65 61	30, 58, 118, 159	3 (0%)
All	All	1217/1226 (99%)	-0.09	20 (1%) 70 67	26, 56, 114, 177	5 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ASN	6.2
1	B	185	LEU	5.7
1	A	187	TRP	4.1
1	B	186	ILE	3.8
1	B	750	VAL	3.6
1	B	198	ALA	3.5
1	B	175	CYS	3.3
1	B	187	TRP	3.2
1	B	174	ALA	3.2
1	A	176	LEU	2.8
1	B	751	PHE	2.7
1	A	439	TRP	2.5
1	B	211	LEU	2.2
1	A	178	LYS	2.2
1	A	211	LEU	2.1
1	B	636	TYR	2.1
1	B	672	HIS	2.1
1	A	399	ARG	2.1
1	A	213	LEU	2.0
1	A	180	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	5	5/5	0.65	0.09	144,144,146,146	0
2	SO4	B	8	5/5	0.67	0.11	118,119,120,121	0
2	SO4	A	4	5/5	0.70	0.12	116,119,121,122	0
3	GOL	A	8	6/6	0.70	0.17	84,89,91,92	0
3	GOL	A	783	6/6	0.78	0.15	87,98,100,102	0
4	MES	B	1	12/12	0.79	0.17	85,91,159,161	0
3	GOL	A	7	6/6	0.82	0.14	87,89,92,93	0
3	GOL	B	6	6/6	0.83	0.16	49,84,91,94	0
2	SO4	B	10	5/5	0.85	0.12	95,103,107,114	0
3	GOL	B	9	6/6	0.88	0.13	77,91,97,104	0
3	GOL	B	3	6/6	0.89	0.10	43,62,68,72	0
3	GOL	B	783	6/6	0.89	0.14	59,73,77,79	0
3	GOL	A	784	6/6	0.90	0.12	46,51,56,61	0
2	SO4	B	7	5/5	0.91	0.07	81,82,93,94	0
2	SO4	A	3	5/5	0.92	0.13	106,107,110,115	0
3	GOL	B	5	6/6	0.93	0.14	41,50,51,55	0
2	SO4	B	2	5/5	0.94	0.06	64,65,72,81	0
2	SO4	A	1	5/5	0.95	0.07	61,62,67,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.